

SIMPLER FORMULAE FOR THE CHAPMAN-COWLING SECOND APPROXIMATION TO THE THERMAL DIFFUSION FACTOR OF BINARY GAS MIXTURES WITH EITHER OF THE COMPONENTS IN TRACE

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Saxena and Dave (1961) have derived simpler formulae for the thermal diffusion factor of a binary gas mixture when the heavier component is in trace. Recently they (1963a, 1963b) also gave the formulae when the lighter component is in trace. Formulae were derived both according to the Chapman-Cowling and Kihara approximation schemes and numerical results were tabulated for the Ar-Xe and He-Xe systems. A critical examination of their work shows that the Chapman-Cowling second approximation formula for thermal diffusion factor, $[\alpha_T]_2$, becomes less accurate as the ratio of the mass of the lighter component to the heavier component increases. In this note we report accurate formulae for such systems.

The new formulae reported here are obtained by applying the following two criteria in expanding the Chapman-Cowling determinants

(i) All the terms in the expansion of the various determinants which contain the product of two diagonal elements of the Chapman-Cowling determinant, $A^{(2)}$, are retained.

(ii) In this expansion those terms are also retained which explicitly contain the power of M upto 2, $M = M_2/M_1$ where M_2 and M_1 are the molecular weights of the lighter and heavier components respectively.

Based on these considerations we get the following expression for $[\alpha_T]_2$ when the heavier component is in trace instead of Eq. (7) of Saxena and Dave (1961).

$$\begin{aligned}
 [\alpha_T]_2 = & (5/2\sqrt{2})(1+M)^{1/2}[(a_{10}/a'_{11}) + M^{-1}\{(a'_{11}a'_{22} - a'_{12}{}^2) \\
 & (a''_{-2-2} a''_{-1-1} - a''_{-1-2}{}^2)\}^{-1}(a'_{11} a'_{22} - a'^2_{12})(a_{-10} a''_{-2-2} - a_{-20} a''_{-1-2}) \\
 & + a_{10}a'_{22}(a''_{-1-2} a_{-21} - a''_{-2-2} a_{-11}) - a''_{-2-2} a_{02} a_{-12} a'_{11}]\}. \quad \dots \quad (1)
 \end{aligned}$$

Similarly when the lighter component is in trace the following formula is obtained instead of Eq. (6) of Saxena and Dave (1963b) :

$$[\alpha_T]_2 = (5/2\sqrt{2})(1 \mp M)^{\frac{1}{2}} \left[a_{10} a''_{22} (a''_{11} a''_{22} - a''_{12}{}^2)^{-1} + \{ (a'_{-1-1} a'_{-2-2} - a'^2_{-1-2}) a'^2_{-1-2} \right. \\ (a''_{11} a''_{22} - a''_{12}{}^2) \}^{-1} \{ (a_{1-1} a''_{22} - a''_{12} a_{2-1}) (a_{-20} a'_{-1-2} - a_{-10} a'_{-2-2}) \\ + (a_{1-2} a''_{22} - a''_{12} a_{2-2}) (a_{-10} a'_{-1-2} - a_{-20} a'_{-1-1}) \} \\ \left. - M^{-\frac{1}{2}} (a_{-10} / a'_{-1-1}) \left(1 - \frac{a_{-20} a'_{-1-2}}{a_{-10} a'_{-2-2}} \right) \left(1 - \frac{a'^2_{-1-2}}{a'_{-1-1} a'_{-2-2}} \right)^{-1} \right]. \quad \dots (2)$$

In both these formulae the various terms have their usual meaning.

TABLE I

Chapman-Cowling calculated values of $[\alpha_T]_2$ for Xe-Ar system, Xe being in trace

| T °K | Rigorous* | S.D. | S.J. |
|---------|-----------|---------|---------|
| 100 | -0.0377 | -0.0428 | -0.0377 |
| 300 | 0.150 | 0.147 | 0.156 |
| 500 | 0.275 | 0.280 | 0.276 |
| 700 | 0.320 | 0.317 | 0.320 |
| 900 | 0.396 | 0.359 | 0.399 |

TABLE II

Chapman-Cowling calculated values of $[\alpha_T]_2$ for Xe-Ar system, Ar in trace

| T °K | Rigorous* | S.D. | S.J. |
|---------|-----------|---------|---------|
| 100 | -0.0234 | -0.0181 | -0.0234 |
| 300 | 0.0894 | 0.0977 | 0.0894 |
| 500 | 0.165 | 0.200 | 0.165 |
| 700 | 0.202 | 0.238 | 0.202 |
| 900 | 0.212 | 0.248 | 0.212 |

*These values are calculated afresh and some differ from those reported earlier by Saxena and Dave.

Computed values of $[\alpha_T]_2$ according to Eqs. 1 and 2 for the Ar-Xe system as a function of temperature are recorded in the last column (S.J.) of Tables I and II respectively. Also included in these tables are the previously reported rigorous (column 2) and approximate (S.D., Column 3) $[\alpha_T]_2$ values. An inspection of these tables reveals that the new formulae given in this note are almost as accurate as the rigorous formulae and are much better than the simpler formulae given earlier by Saxena and Davo (1961, 1963a, and 1963b). These new formulae will be extremely useful for predicting the $[\alpha_T]_2$ values or in determining the inter-molecular forces if α_T experimental data are available for those systems where M is not quite small.

It may be pointed out that this method of approximating the Chapman-Cowling determinants has proved very successful for the general case of α_T where both the components are present in appreciable proportions, (Saxena, Dave and Pardeshi 1962, Saxena and Joshi 1963a) and also in the formulation of the second approximation to the binary viscosity (Saxena and Joshi, 1963b)

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